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The Finite-Volume-Particle Method for Conservation Laws

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Vorwort

Das Tätigkeitsfeld des Fraunhofer Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe sollen sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen werden.

Darüberhinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation darüber, wie aktuelle Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte transferiert werden, und wie umgekehrt Probleme der Praxis neue interessante mathematische Fragestellungen generieren.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

The Finite-Volume-Particle Method for Conservation Laws

D. Hietel* M. Junk† R. Keck* D. Teleaga‡

7th December 2000

Abstract

In the Finite-Volume-Particle Method (FVPM), the weak formulation of a hyperbolic conservation law is discretized by restricting it to a discrete set of test functions. In contrast to the usual Finite-Volume approach, the test functions are not taken as characteristic functions of the control volumes in a spatial grid, but are chosen from a partition of unity with smooth and overlapping partition functions (the particles), which can even move along prescribed velocity fields. The information exchange between particles is based on standard numerical flux functions. Geometrical information, similar to the surface area of the cell faces in the Finite-Volume Method and the corresponding normal directions are given as integral quantities of the partition functions.

After a brief derivation of the Finite-Volume-Particle Method, this work focuses on the role of the geometric coefficients in the scheme.

1 Introduction

The Finite-Volume-Particle Method (FVPM) is a new mesh-less method for the discretization of conservation laws. The motivation for developing a new method is to unify advantages of particle methods and Finite-Volume Methods (FVM) in one scheme.

On the one hand, particle methods are very flexible because they are mesh-free. The need for mesh-less methods typically arises if problems with time dependent or very complicated geometries are under consideration because then

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the handling of mesh discretizations becomes technically complicated or very time consuming. Fluid flow with structural interaction or fast moving boundaries like an inflating air-bag are of that kind for instance.

In gas and fluid dynamics, the SPH method [Mon92] has been successfully applied to problems with free boundaries. Recent developments in the area of mesh-less methods include the Finite-Mass Method (FMM) [Yse97, GLY] and the partition of unity method (PUM) [GS00].

The basic idea in the FVPM is to incorporate elements of the FVM into a particle method. Specifically, one wants to adopt the treatment of boundary conditions and the FVM concept of numerical flux functions in order to avoid numerical fit-parameters as in the artificial viscosity terms of SPH.

The brief derivation of the Finite-Volume-Particle Method in the following section shows that the scheme is essentially determined by the numerical flux function and a set of geometrical coefficients which play the role of normal directions and surface areas of cell faces in the Finite-Volume Method. For one-dimensional, scalar conservation laws, a Lax-Wendroff type consistency analysis and stability requirements lead to a set of conditions on the coefficients. For example, a CFL-type condition assures monotonicity of the scheme if the underlying numerical flux function is monotone. Numerical examples are presented to show the behavior of the scheme in the case of Burgers' equation. The extension to two-dimensional cases is demonstrated for the system of Euler equations. For certain 2D shock tube problems, it is shown how the identification of the geometric coefficients with their Finite-Volume counterparts (i.e. normal directions and length of cell faces) allows the implementation of boundary conditions.

2 Derivation of the scheme

In the following, we will briefly summarize the derivation of FVPM which was developed in [HSS]. As already mentioned above, FVPM is a numerical method for solving conservation laws of the type

$$\frac{\partial}{\partial t}\boldsymbol{\Phi}(t,\boldsymbol{x}) + \nabla \cdot \boldsymbol{F}(\boldsymbol{\Phi}(t,\boldsymbol{x})) = \boldsymbol{0}, \qquad \forall \boldsymbol{x} \in \Omega \subset \mathbb{R}^d,\ t \in \mathbb{R}^+ \tag{1}$$

with accompanying boundary and initial conditions $\boldsymbol{\Phi}(0,\boldsymbol{x}) = \boldsymbol{\Phi}^{(0)}(\boldsymbol{x})$. Here, $\boldsymbol{\Phi}$ denotes the vector of conservative variables, $\boldsymbol{F}$ is the flux function of the conservation law, d is the spatial dimension, and Ω is the domain under consideration.

A natural approach to discretize conservation laws is to evaluate the weak formulation with a discrete set of test functions $\psi_i, i = 1,..,N$. In classical Finite-Volume Methods, the test functions are taken as characteristic functions $\psi_i(\boldsymbol{x}) := \mathbb{I}_{\nu_i}(\boldsymbol{x})$ of the control volumes ν_i in a spatial grid. Note that the test functions form a *partition of unity*, i.e. $\sum_{i=1}^{N} \psi_i(\boldsymbol{x}) \equiv 1$, $\forall \boldsymbol{x} \in \Omega$.

In contrast to that, *smooth* test functions ψ_i (called *particles*) are employed in the FVPM. More precisely, at the *particle positions* $\boldsymbol{x}_i(t)$, the construction of ψ_i is based on a compactly supported smoothing kernel $W(\boldsymbol{x})$, as it is used, for example, in the SPH method. The functions $W_i(\boldsymbol{x}) = W(\boldsymbol{x} - \boldsymbol{x}_i(t))$ are then re-normalized by the particle-density $\sigma(x)$, according to Shepard's method

$$\psi_i(t, \boldsymbol{x}) := \frac{W(\boldsymbol{x} - \boldsymbol{x}_i(t))}{\sigma(t, \boldsymbol{x})}, \quad \text{where} \quad \sigma(t, \boldsymbol{x}) := \sum_{j=1}^{N} W(\boldsymbol{x} - \boldsymbol{x}_j(t)).$$

For an illustration of the construction of the test functions ψ_i see Figures 1 to 3. Due to Shepard's re-normalization, the particles form a *partition of unity*

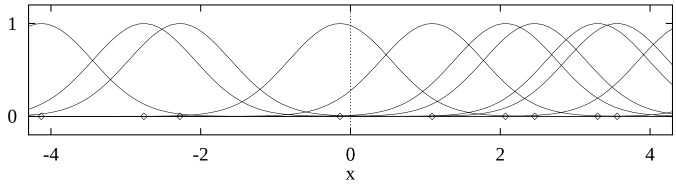

Figure 1: Irregular particle positions x_i and functions $W_i(x) = W(x - x_i)$

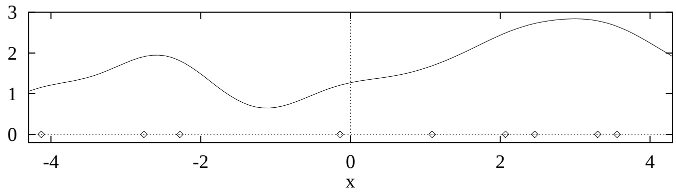

Figure 2: The function $\sigma(x) = \sum_i W_i(x)$ corresponding to Fig. 1

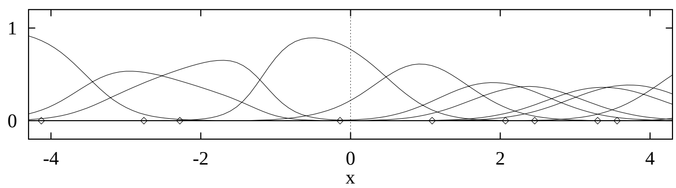

Figure 3: The resulting partition of unity $\psi_i(x) = W_i(x)/\sigma(x)$

similar to the characteristic functions of the control-volumes in the FVM. In Figure 3, one can see that the resulting test functions are scaled according to the particle-density, i.e. in regions where the particle-density is high the corresponding test functions are small which means small local weights of the corresponding particles.

In the FVPM, the particles generically move through the domain, following the 'arbitrary' velocity vectors $\boldsymbol{u}_i$, i.e. $\dot{\boldsymbol{x}}_i = \boldsymbol{u}_i$. For $\boldsymbol{u} = \boldsymbol{0}$, one obtains fixed particles and for $\boldsymbol{u}$ being, for example, the fluid velocity in the case of Euler equations, one obtains a Lagrangian scheme.

To each particle, one associates a volume V_i and a discrete quantity $\boldsymbol{\Phi}_i$ which is the integral mean value with respect to the test function

$$\boldsymbol{\Phi}_i(t,\boldsymbol{x}) := \frac{1}{V_i}\int\limits_{\Omega} \boldsymbol{\Phi}(t,\boldsymbol{x})\psi_i(t,\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \quad \text{where} \quad V_i(t) := \int\limits_{\Omega} \psi_i(t,\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

Using the test functions and quantities defined above, one obtains the following evolution equations for the discrete quantities from the weak formulation of the Cauchy problem (1) (see [HSS] for details):

$$\frac{d}{dt}\left(V_i\boldsymbol{\Phi}_i\right) = -\sum_{j=1}^{N} |\boldsymbol{\beta}_{ij}|\tilde{\boldsymbol{F}}\left(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_j; \frac{\boldsymbol{\beta}_{ij}}{|\boldsymbol{\beta}_{ij}|}\right) + \sum_{j=1}^{N}\left(\boldsymbol{\gamma}_{ij}\cdot\dot{\boldsymbol{x}}_j\boldsymbol{\Phi}_i - \boldsymbol{\gamma}_{ji}\cdot\dot{\boldsymbol{x}}_i\boldsymbol{\Phi}_j\right), \quad (2)$$

together with

$$\frac{d}{dt}V_i = \sum_{j=1}^{N}\left(\boldsymbol{\gamma}_{ij}\cdot\dot{\boldsymbol{x}}_j - \boldsymbol{\gamma}_{ji}\cdot\dot{\boldsymbol{x}}_i\right), \qquad \frac{d}{dt}\boldsymbol{x}_i = \boldsymbol{u}_i.$$

The coefficients $\boldsymbol{\gamma}_{ij}$ and $\boldsymbol{\beta}_{ij}$ are defined as

$$\boldsymbol{\beta}_{ij} := \boldsymbol{\gamma}_{ij} - \boldsymbol{\gamma}_{ji}, \quad \boldsymbol{\gamma}_{ij} := \int \psi_i \frac{\nabla W_j}{\sigma}\,\mathrm{d}\boldsymbol{x}. \quad (3)$$

The right hand side of the evolution equation (2) consists of two parts. The first part is the flux term, where a standard numerical flux function $\tilde{\boldsymbol{F}}$ may be used, and the second term corresponds to the movement of the particles.

We remark that the formulation (2) may suffer from instabilities as can be seen by applying the discretization to the trivial scalar conservation law

$$\frac{\partial\Phi}{\partial t} = 0, \qquad \Phi(0,x) = H(x), \quad x\in\mathbb{R}$$

where H is the Heaviside function. We use the numerical flux $\tilde{F}\equiv 0$ and equidistant particles at $x_i = ih$, $i\in\mathbb{Z}$ which move with a common speed $\dot{x}_i = -1$. The hat function $W(x) = (1-|x/h|)_+$ then gives rise to $\psi_i(t,x) = W(x - x_i(t))$ since $\sigma\equiv 1$. With these choices, the scheme (2) reduces to

$$\frac{d\Phi_i}{dt} + \frac{\Phi_{i+1}-\Phi_{i-1}}{2h} = 0$$

which leads to the unconditionally unstable central scheme if the time derivative is discretized with a forward Euler method. Note that the central difference has its origin in the second sum in (2) which reflects corrections due to the movement of the particles.

A more stable discretization has been proposed in [JS00] where the movement terms are incorporated into the flux function, leading to a scheme of the form

$$\frac{d}{dt}\left(V_i \boldsymbol{\Phi}_i\right) = -\sum_{j=1}^{N} |\boldsymbol{\beta}_{ij}| \boldsymbol{G}_{ij} \tag{4}$$

where $\boldsymbol{G}_{ij}$ is a numerical flux function which corresponds to the modified flux $\boldsymbol{G}(t, \boldsymbol{x}, \boldsymbol{\Phi}) = \boldsymbol{F}(\boldsymbol{\Phi}) - \boldsymbol{\Phi} \otimes \boldsymbol{u}$. Selecting for example a flux function based on upwind ideas, we conclude that the example $\boldsymbol{F} \equiv \boldsymbol{0}$ no longer leads to instabilities since the movement terms are now treated properly.

3 The coefficients of the scheme

3.1 Formal aspects of the coefficients

The behavior of the FVPM is significantly influenced by the coefficients $\boldsymbol{\gamma}_{ij}$ and $\boldsymbol{\beta}_{ij}$ defined in (3). In order to analyze the effect of the coefficients, we consider the scheme (4) for scalar valued equations in $\Omega = \mathbb{R}$. Proofs for the results can be found in [HSS, JS00, Tel00].

A symmetry condition of the form

$$\beta_{ij} = -\beta_{ji} \tag{5}$$

ensures that the scheme is conservative, i.e. that $\frac{d}{dt}\left(\sum_i V_i \boldsymbol{\Phi}_i\right) = 0$. Monotonicity of the scheme follows under a CFL-like condition on the time-step if a monotone numerical flux function is used

$$L \frac{\Delta t}{\mathsf{min}_i V_i} < \frac{1}{\mathsf{max}_i \sum_j |\beta_{ij}|}. \tag{6}$$

Here, L is the Lipschitz constant for the numerical flux function which is related to the maximal characteristic speed in the problem. Furthermore, monotonicity and a summation condition of the form

$$\sum_{j \in \mathbb{Z}} \beta_{ij} = 0, \forall i \in \mathbb{Z}, \tag{7}$$

give $\mathbb{L}^\infty$-stability for finite times $0 \leq t \leq T$

$$\|\sum_i \Phi_i(t)\psi_i\|_{\mathbb{L}^\infty} \leq e^{CT} \|\sum_i \Phi_i(0)\psi_i\|_{\mathbb{L}^\infty}. \tag{8}$$

If the coefficients additionally satisfy a summation condition of the form

$$\sum_{i \geq i_0} \sum_{j \geq i_0} \beta_{ij} = 1 \tag{9}$$

the scheme is consistent in the sense of Lax-Wendroff, i.e. if the approximate solutions converge in a suitable sense, they converge to a weak solution.

An estimate for the total variation is in preparation and seems to be achievable under the conditions (6) and (7). To finally get convergence of the scheme to the entropy-solution, an entropy inequality is required.

We remark that conditions (7) and (9) are difficult to ensure if the integrals in (3) are evaluated numerically and that violation of these conditions may lead to instabilities of the method. To illustrate, for example, the effect of the summation-condition (7) on the scheme we consider a standard Riemann problem for Burgers' equation. In the left plot of Figure 4, the summation condition (7) is not fulfilled, which leads to unphysical oscillations in the constant part of the solution. In the right plot, the condition is satisfied and the oscillations vanish (see [Tel00] for the proof). Since highly accurate numerical integration is

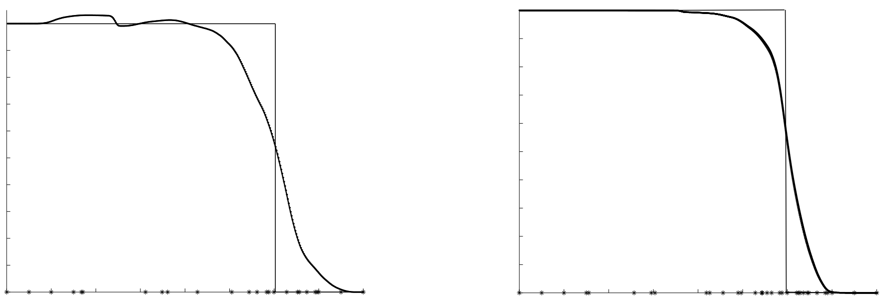

Figure 4: The effect of the summation condition (7) on the solution.

very time consuming, the determination of the coefficients turns out to be the most expensive part of the scheme. To alleviate this problem, a method has been proposed in [Tel00] which is based on a coarse evaluation of the integrals and a subsequent correction procedure in order to ensure (5), (7), and (9). However, this method is still at an experimental stage.

3.2 Heuristic interpretation of the coefficients

According to the definition (3), the coefficients $\boldsymbol{\beta}_{ij}$ are averaged, weighted, and symmetrized gradients of the smoothing kernels. This interpretation is illustrated in Figure 5. A formal comparison with standard Finite-Volume Methods (see (10) and (11)) indicates that the coefficients $|\boldsymbol{\beta}_{ij}|$ and $\boldsymbol{\beta}_{ij}/|\boldsymbol{\beta}_{ij}|$ can be interpreted as generalized surface area $|S_{ij}|$ of cell faces in the FVM and the corresponding

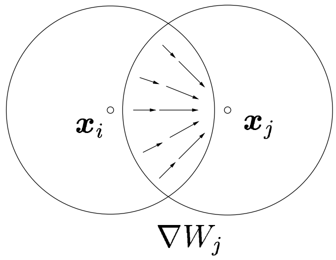

Figure 5: The gradient of the smoothing kernel: ∇W_j.

normal directions $\boldsymbol{\nu}_{ij}$:

$$\frac{d}{dt}(V_i\boldsymbol{\Phi}_i) = -\sum_j |\boldsymbol{\beta}_{ij}|\tilde{\boldsymbol{F}}\left(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_j, \frac{\boldsymbol{\beta}_{ij}}{|\boldsymbol{\beta}_{ij}|}\right) \quad \mathsf{FVPM} \;\; (\dot{\boldsymbol{x}}_i = \boldsymbol{0}), \tag{10}$$

$$\frac{d}{dt}(V_i\boldsymbol{\Phi}_i) = -\sum_j |S_{ij}|\tilde{\boldsymbol{F}}(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_j, \boldsymbol{\nu}_{ij}) \quad \mathsf{FVM}. \tag{11}$$

These considerations indicate that the Finite-Volume-Particle Method is in some sense a 'generalization' of the standard Finite-Volume Method. In fact, the use of smooth and overlapping test functions (in contrast to the characteristic functions in the FVM) can be interpreted as a generalization of FVM to overlapping, smoothed, and moving control volumes.

4 Numerical results

The validation of the scheme is done by solving a standard and a modified 2D shock tube problem for the Euler equations of gas dynamics with free-slip boundary conditions.

4.1 Boundary treatment

The boundary treatment of the FVPM consists of two parts: Firstly, the boundary interacts with a particle by cutting off the support of the test function in definition (3) of the coefficients $\boldsymbol{\gamma}_{ij}$. Secondly, free-slip boundary-conditions are implemented using boundary-fluxes similar to the FVM.

The boundary-fluxes are computed using the normal $\boldsymbol{n}_i$ and the tangential vector $\boldsymbol{t}_i$ of the boundary at the corresponding particle $\boldsymbol{x}_i$ and the numerical flux function $\tilde{\boldsymbol{F}}(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_j; \boldsymbol{n}_i)$ which is used in the scheme. The auxiliary state $\boldsymbol{\Phi}_j$ is computed so that the boundary conditions are satisfied:

$$\boldsymbol{u}_i \cdot \boldsymbol{n}_i = -\boldsymbol{u}_j \cdot \boldsymbol{n}_i, \qquad \boldsymbol{u}_i \cdot \boldsymbol{t}_i = \boldsymbol{u}_j \cdot \boldsymbol{t}_i.$$

4.2 Quasi-1D shock tube problem

As initial condition, a density and pressure ratio of $1/10$ across an initial shock at $x = 0.55$ in the domain $[0, 1] \times [0, 0.1]$ has been chosen. The shock front travels towards the right wall where it is reflected. The calculation is based on 1 000 particles (100 in x-direction and 10 in y-direction).

In Figure 6 a cut through the domain is shown. The density of the particles is plotted over the x-component of the position at time $t = 0.2$ and $t = 0.6$ in the left and right plot, respectively. Reflection of the shock wave at the right wall has already taken place in the right plot.

The simulation shows that the implementation of the boundary conditions works very satisfactory. No boundary effects are visible because all cuts through the domain give the same result.

In order to avoid holes in the computational domain by the movement of the particles, the radius of the particle support is chosen as $h = 1.8\Delta x$, where Δx denotes the initial distance between particle positions in x-direction.

Comparing FVPM and FVM based on the same flux function (Roe's flux), we find that despite the considerable overlap of the particles, the FVPM-solution turns out to be almost as accurate as the FVM-solution on a fixed 100×10 grid (spacing Δx) and it is notably better than the FVM-solution on a grid with spacing $2h$.

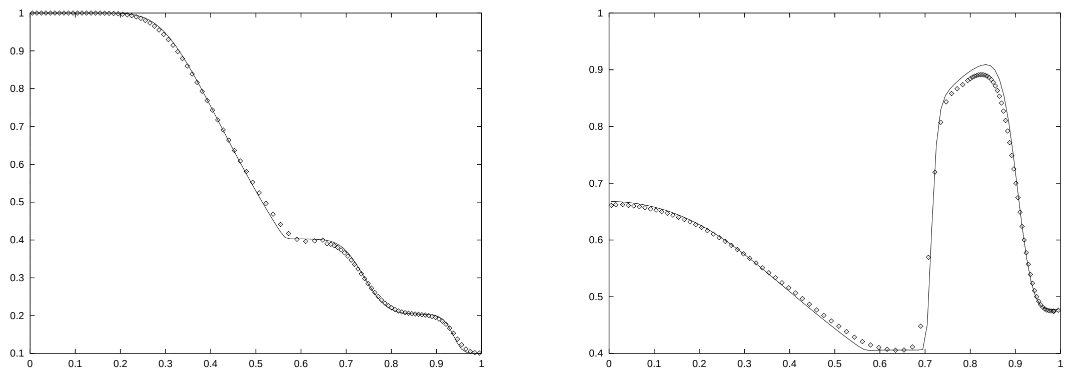

Figure 6: Solution of the standard shock-tube problem (density). Left: Before the shock front reaches the right wall at $t = 0.2$. Right: After reflection at the right wall at $t = 0.6$. The solid line is a FVM-solution on a 100×10 grid.

4.3 Modified shock tube problem

In the modified problem a quadratic domain is considered and the discontinuity in the initial data is located along the diagonal of the domain $x = y$. The shock front travels towards the upper left corner where it is reflected. Figure 7 shows the density and the velocity field shortly after reflection. The computation was performed on a domain $[0, 20] \times [0, 20]$ with 10 000 particles.

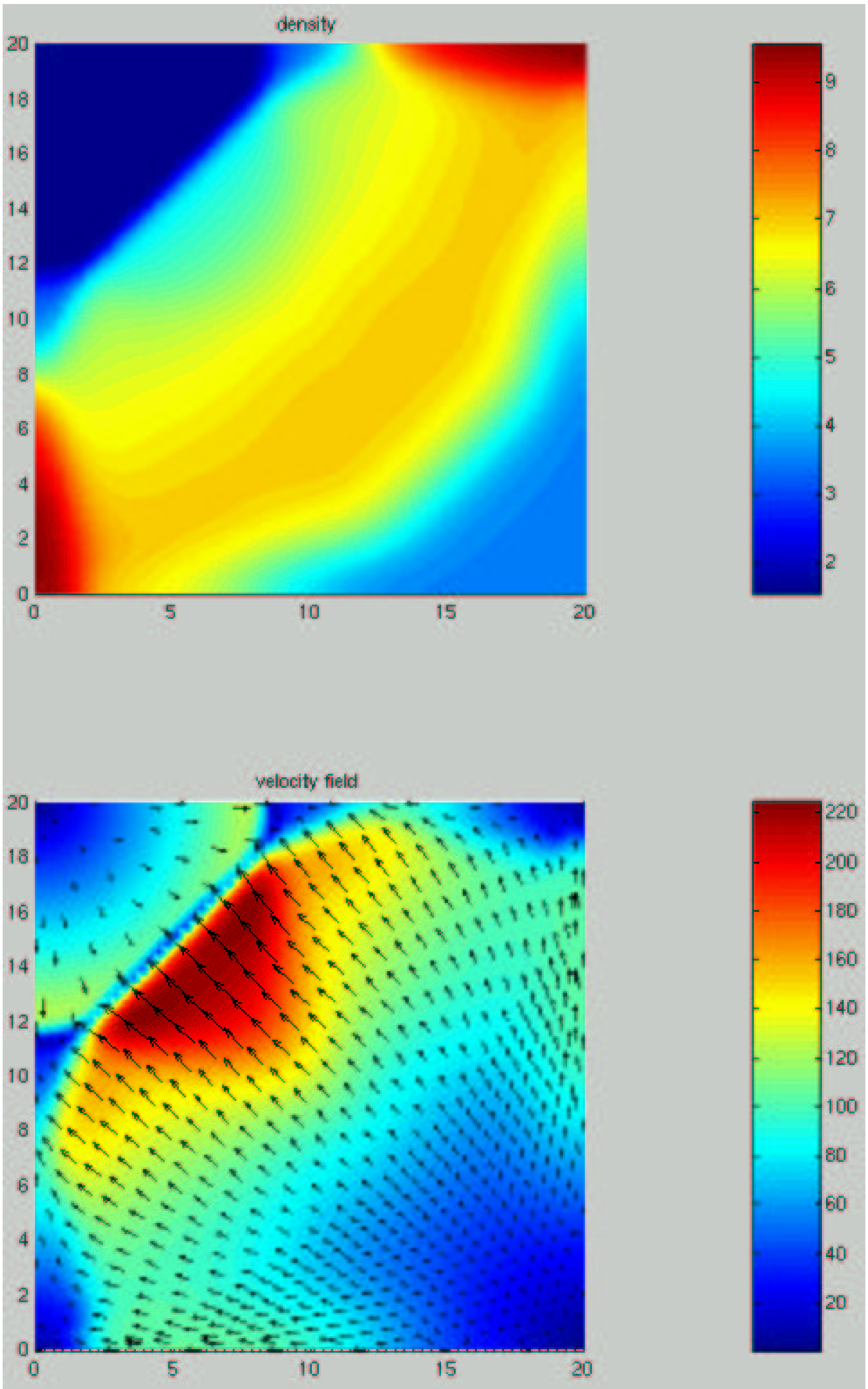

Figure 7: Solution of the shock problem after reflection in the upper left corner.

References

[GLY] C. Gauger, P. Leinen, and H. Yserentant. The finite mass method. *To appear in SIAM Journal on Numerical Analysis.*

[GS00] M. Griebel and M. A. Schweitzer. A particle-partition of unity method for the solution of elliptic, parabolic and hyperbolic pdes. *SIAM Journal on Scientific Computing*, 2000.

[HSS] D. Hietel, K. Steiner, and J. Struckmeier. A finite-volume particle method for compressible flows. *To appear in Mathematical Models and Methods in Applied Science.*

[JS00] M. Junk and J. Struckmeier. Consistency analysis of mesh-free methods for conservation laws. *Berichte der AG Technomathematik, Universität Kaiserslautern*, 226, 2000.

[Mon92] J. J. Monaghan. Smoothed particle hydrodynamics. *Annual Review of Astronomy and Astrophysics*, 30:543–574, 1992.

[Tel00] D. Teleaga. *Numerical Studies of a Finite-Volume Particle Method for Conservation Laws.* Master Thesis, Department of Mathematics, Universität Kaiserslautern, 2000.

[Yse97] H. Yserentant. A particle method of compressible fluids. *Numerische Mathematik*, 76:111–142, 1997.

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1. D. Hietel, K. Steiner, J. Struckmeier

A Finite - Volume Particle Method for Compressible Flows

We derive a new class of particle methods for conservation laws, which are based on numerical flux functions to model the interactions between moving particles. The derivation is similar to that of classical Finite-Volume methods; except that the fixed grid structure in the Finite-Volume method is substituted by so-called mass packets of particles. We give some numerical results on a shock wave solution for Burgers equation as well as the well-known one-dimensional shock tube problem.
(19 S., 1998)

2. M. Feldmann, S. Seibold

Damage Diagnosis of Rotors: Application of Hilbert Transform and Multi-Hypothesis Testing

In this paper, a combined approach to damage diagnosis of rotors is proposed. The intention is to employ signal-based as well as model-based procedures for an improved detection of size and location of the damage. In a first step, Hilbert transform signal processing techniques allow for a computation of the signal envelope and the instantaneous frequency, so that various types of non-linearities due to a damage may be identified and classified based on measured response data. In a second step, a multi-hypothesis bank of Kalman Filters is employed for the detection of the size and location of the damage based on the information of the type of damage provided by the results of the Hilbert transform.
Keywords:
Hilbert transform, damage diagnosis, Kalman filtering, non-linear dynamics
(23 S., 1998)

3. Y. Ben-Haim, S. Seibold

Robust Reliability of Diagnostic Multi-Hypothesis Algorithms: Application to Rotating Machinery

Damage diagnosis based on a bank of Kalman filters, each one conditioned on a specific hypothesized system condition, is a well recognized and powerful diagnostic tool. This multi-hypothesis approach can be applied to a wide range of damage conditions. In this paper, we will focus on the diagnosis of cracks in rotating machinery. The question we address is: how to optimize the multi-hypothesis algorithm with respect to the uncertainty of the spatial form and location of cracks and their resulting dynamic effects. First, we formulate a measure of the reliability of the diagnostic algorithm, and then we discuss modifications of the diagnostic algorithm for the maximization of the reliability. The reliability of a diagnostic algorithm is measured by the amount of uncertainty consistent with no-failure of the diagnosis. Uncertainty is quantitatively represented with convex models.
Keywords:
Robust reliability, convex models, Kalman filtering, multi-hypothesis diagnosis, rotating machinery, crack diagnosis
(24 S., 1998)

4. F.-Th. Lentes, N. Siedow

Three-dimensional Radiative Heat Transfer in Glass Cooling Processes

For the numerical simulation of 3D radiative heat transfer in glasses and glass melts, practically applicable mathematical methods are needed to handle such problems optimal using workstation class computers. Since the exact solution would require super-computer capabilities we concentrate on approximate solutions with a high degree of accuracy. The following approaches are studied: 3D diffusion approximations and 3D ray-tracing methods.
(23 S., 1998)

5. A. Klar, R. Wegener

A hierarchy of models for multilane vehicular traffic
Part I: Modeling

In the present paper multilane models for vehicular traffic are considered. A microscopic multilane model based on reaction thresholds is developed. Based on this model an Enskog like kinetic model is developed. In particular, care is taken to incorporate the correlations between the vehicles. From the kinetic model a fluid dynamic model is derived. The macroscopic coefficients are deduced from the underlying kinetic model. Numerical simulations are presented for all three levels of description in [10]. Moreover, a comparison of the results is given there.
(23 S., 1998)

Part II: Numerical and stochastic investigations

In this paper the work presented in [6] is continued. The present paper contains detailed numerical investigations of the models developed there. A numerical method to treat the kinetic equations obtained in [6] are presented and results of the simulations are shown. Moreover, the stochastic correlation model used in [6] is described and investigated in more detail.
(17 S., 1998)

6. A. Klar, N. Siedow

Boundary Layers and Domain Decomposition for Radiative Heat Transfer and Diffusion Equations: Applications to Glass Manufacturing Processes

In this paper domain decomposition methods for radiative transfer problems including conductive heat transfer are treated. The paper focuses on semi-transparent materials, like glass, and the associated conditions at the interface between the materials. Using asymptotic analysis we derive conditions for the coupling of the radiative transfer equations and a diffusion approximation. Several test cases are treated and a problem appearing in glass manufacturing processes is computed. The results clearly show the advantages of a domain decomposition approach. Accuracy equivalent to the solution of the global radiative transfer solution is achieved, whereas computation time is strongly reduced.
(24 S., 1998)

7. I. Choquet

Heterogeneous catalysis modelling and numerical simulation in rarified gas flows
Part I: Coverage locally at equilibrium

A new approach is proposed to model and simulate numerically heterogeneous catalysis in rarefied gas flows. It is developed to satisfy all together the following points:
1) describe the gas phase at the microscopic scale, as required in rarefied flows,
2) describe the wall at the macroscopic scale, to avoid prohibitive computational costs and consider not only crystalline but also amorphous surfaces,
3) reproduce on average macroscopic laws correlated with experimental results and
4) derive analytic models in a systematic and exact way.
The problem is stated in the general framework of a non static flow in the vicinity of a catalytic and non porous surface (without aging). It is shown that the exact and systematic resolution method based on the Laplace transform, introduced previously by the author to model collisions in the gas phase, can be extended to the present problem. The proposed approach is applied to the modelling of the Eley-Rideal and Langmuir-Hinshelwood recombinations, assuming that the coverage is locally at equilibrium. The models are developed considering one atomic species and extended to the general case of several atomic species. Numerical calculations show that the models derived in this way reproduce with accuracy behaviors observed experimentally.
(24 S., 1998)

8. J. Ohser, B. Steinbach, C. Lang

Efficient Texture Analysis of Binary Images

A new method of determining some characteristics of binary images is proposed based on a special linear filtering. This technique enables the estimation of the area fraction, the specific line length, and the specific integral of curvature. Furthermore, the specific length of the total projection is obtained, which gives detailed information about the texture of the image. The influence of lateral and directional resolution depending on the size of the applied filter mask is discussed in detail. The technique includes a method of increasing directional resolution for texture analysis while keeping lateral resolution as high as possible.
(17 S., 1998)

9. J. Orlik

Homogenization for viscoelasticity of the integral type with aging and shrinkage

A multi-phase composite with periodic distributed inclusions with a smooth boundary is considered in this contribution. The composite component materials are supposed to be linear viscoelastic and aging (of the non-convolution integral type, for which the Laplace transform with respect to time is not effectively applicable) and are subjected to isotropic shrinkage. The free shrinkage deformation can be considered as a fictitious temperature deformation in the behavior law. The procedure presented in this paper proposes a way to determine average (effective homogenized) viscoelastic and shrinkage (temperature) composite properties and the homogenized stress-field from known properties of the

components. This is done by the extension of the asymptotic homogenization technique known for pure elastic non-homogeneous bodies to the non-homogeneous thermo-viscoelasticity of the integral non-convolution type. Up to now, the homogenization theory has not covered viscoelasticity of the integral type.
Sanchez-Palencia (1980), Francfort & Suquet (1987) (see [2], [9]) have considered homogenization for viscoelasticity of the differential form and only up to the first derivative order. The integral-modeled viscoelasticity is more general then the differential one and includes almost all known differential models. The homogenization procedure is based on the construction of an asymptotic solution with respect to a period of the composite structure. This reduces the original problem to some auxiliary boundary value problems of elasticity and viscoelasticity on the unit periodic cell, of the same type as the original non-homogeneous problem. The existence and uniqueness results for such problems were obtained for kernels satisfying some constrain conditions. This is done by the extension of the Volterra integral operator theory to the Volterra operators with respect to the time, whose 1 kernels are space linear operators for any fixed time variables. Some ideas of such approach were proposed in [11] and [12], where the Volterra operators with kernels depending additionally on parameter were considered. This manuscript delivers results of the same nature for the case of the space-operator kernels.
(20 S., 1998)

10. J. Mohring
Helmholtz Resonators with Large Aperture

The lowest resonant frequency of a cavity resonator is usually approximated by the classical Helmholtz formula. However, if the opening is rather large and the front wall is narrow this formula is no longer valid. Here we present a correction which is of third order in the ratio of the diameters of aperture and cavity. In addition to the high accuracy it allows to estimate the damping due to radiation. The result is found by applying the method of matched asymptotic expansions. The correction contains form factors describing the shapes of opening and cavity. They are computed for a number of standard geometries. Results are compared with numerical computations.
(21 S., 1998)

11. H. W. Hamacher, A. Schöbel
On Center Cycles in Grid Graphs

Finding "good" cycles in graphs is a problem of great interest in graph theory as well as in locational analysis. We show that the center and median problems are NP hard in general graphs. This result holds both for the variable cardinality case (i.e. all cycles of the graph are considered) and the fixed cardinality case (i.e. only cycles with a given cardinality p are feasible). Hence it is of interest to investigate special cases where the problem is solvable in polynomial time.
In grid graphs, the variable cardinality case is, for instance, trivially solvable if the shape of the cycle can be chosen freely.
If the shape is fixed to be a rectangle one can analyze rectangles in grid graphs with, in sequence, fixed dimension, fixed cardinality, and variable cardinality. In all cases a complete characterization of the optimal cycles and closed form expressions of the optimal objective values are given, yielding polynomial time algorithms for all cases of center rectangle problems.
Finally, it is shown that center cycles can be chosen as rectangles for small cardinalities such that the center cycle problem in grid graphs is in these cases completely solved.
(15 S., 1998)

12. H. W. Hamacher, K.-H. Küfer
Inverse radiation therapy planning - a multiple objective optimisation approach

For some decades radiation therapy has been proved successful in cancer treatment. It is the major task of clinical radiation treatment planning to realize on the one hand a high level dose of radiation in the cancer tissue in order to obtain maximum tumor control. On the other hand it is obvious that it is absolutely necessary to keep in the tissue outside the tumor, particularly in organs at risk, the unavoidable radiation as low as possible.
No doubt, these two objectives of treatment planning - high level dose in the tumor, low radiation outside the tumor - have a basically contradictory nature. Therefore, it is no surprise that inverse mathematical models with dose distribution bounds tend to be infeasible in most cases. Thus, there is need for approximations compromising between overdosing the organs at risk and underdosing the target volume.
Differing from the currently used time consuming iterative approach, which measures deviation from an ideal (non-achievable) treatment plan using recursively trial-and-error weights for the organs of interest, we go a new way trying to avoid a priori weight choices and consider the treatment planning problem as a multiple objective linear programming problem: with each organ of interest, target tissue as well as organs at risk, we associate an objective function measuring the maximal deviation from the prescribed doses.
We build up a data base of relatively few efficient solutions representing and approximating the variety of Pareto solutions of the multiple objective linear programming problem. This data base can be easily scanned by physicians looking for an adequate treatment plan with the aid of an appropriate online tool.
(14 S., 1999)

13. C. Lang, J. Ohser, R. Hilfer
On the Analysis of Spatial Binary Images

This paper deals with the characterization of microscopically heterogeneous, but macroscopically homogeneous spatial structures. A new method is presented which is strictly based on integral-geometric formulae such as Crofton's intersection formulae and Hadwiger's recursive definition of the Euler number. The corresponding algorithms have clear advantages over other techniques. As an example of application we consider the analysis of spatial digital images produced by means of Computer Assisted Tomography.
(20 S., 1999)

14. M. Junk
On the Construction of Discrete Equilibrium Distributions for Kinetic Schemes

A general approach to the construction of discrete equilibrium distributions is presented. Such distribution functions can be used to set up Kinetic Schemes as well as Lattice Boltzmann methods. The general principles are also applied to the construction of Chapman Enskog distributions which are used in Kinetic Schemes for compressible Navier-Stokes equations.
(24 S., 1999)

15. M. Junk, S. V. Raghurame Rao
A new discrete velocity method for Navier-Stokes equations

The relation between the Lattice Boltzmann Method, which has recently become popular, and the Kinetic Schemes, which are routinely used in Computational Fluid Dynamics, is explored. A new discrete velocity model for the numerical solution of Navier-Stokes equations for incompressible fluid flow is presented by combining both the approaches. The new scheme can be interpreted as a pseudo-compressibility method and, for a particular choice of parameters, this interpretation carries over to the Lattice Boltzmann Method.
(20 S., 1999)

16. H. Neunzert
Mathematics as a Key to Key Technologies

The main part of this paper will consist of examples, how mathematics really helps to solve industrial problems; these examples are taken from our Institute for Industrial Mathematics, from research in the Technomathematics group at my university, but also from ECMI groups and a company called TecMath, which originated 10 years ago from my university group and has already a very successful history.
(39 S. (vier PDF-Files), 1999)

17. J. Ohser, K. Sandau
Considerations about the Estimation of the Size Distribution in Wicksell's Corpuscle Problem

Wicksell's corpuscle problem deals with the estimation of the size distribution of a population of particles, all having the same shape, using a lower dimensional sampling probe. This problem was originary formulated for particle systems occurring in life sciences but its solution is of actual and increasing interest in materials science. From a mathematical point of view, Wicksell's problem is an inverse problem where the interesting size distribution is the unknown part of a Volterra equation. The problem is often regarded ill-posed, because the structure of the integrand implies unstable numerical solutions. The accuracy of the numerical solutions is considered here using the condition number, which allows to compare different numerical methods with different (equidistant) class sizes and which indicates, as one result, that a finite section thickness of the probe reduces the numerical problems. Furthermore, the relative error of estimation is computed which can be split into two parts. One part consists of the relative discretization error that increases for increasing class size, and the second part is related to the relative statistical error which increases with decreasing class size. For both parts, upper bounds can be given and the sum of them indicates an optimal class width depending on some specific constants.
(18 S., 1999)

18. E. Carrizosa, H. W. Hamacher, R. Klein, S. Nickel

Solving nonconvex planar location problems by finite dominating sets

It is well-known that some of the classical location problems with polyhedral gauges can be solved in polynomial time by finding a finite dominating set, i. e. a finite set of candidates guaranteed to contain at least one optimal location.
In this paper it is first established that this result holds for a much larger class of problems than currently considered in the literature. The model for which this result can be proven includes, for instance, location problems with attraction and repulsion, and location-allocation problems.
Next, it is shown that the approximation of general gauges by polyhedral ones in the objective function of our general model can be analyzed with regard to the subsequent error in the optimal objective value. For the approximation problem two different approaches are described, the sandwich procedure and the greedy algorithm. Both of these approaches lead - for fixed epsilon - to polynomial approximation algorithms with accuracy epsilon for solving the general model considered in this paper.
Keywords:
Continuous Location, Polyhedral Gauges, Finite Dominating Sets, Approximation, Sandwich Algorithm, Greedy Algorithm
(19 S., 2000)

19. A. Becker

A Review on Image Distortion Measures

Within this paper we review image distortion measures. A distortion measure is a criterion that assigns a "quality number" to an image. We distinguish between mathematical distortion measures and those distortion measures in-cooperating a priori knowledge about the imaging devices (e. g. satellite images), image processing algorithms or the human physiology. We will consider representative examples of different kinds of distortion measures and are going to discuss them.
Keywords:
Distortion measure, human visual system
(26 S., 2000)

20. H. W. Hamacher, M. Labbé, S. Nickel, T. Sonneborn

Polyhedral Properties of the Uncapacit*ated Multiple Allocation Hub Location Problem*

We examine the feasibility polyhedron of the uncapacitated hub location problem (UHL) with multiple allocation, which has applications in the fields of air passenger and cargo transportation, telecommunication and postal delivery services. In particular we determine the dimension and derive some classes of facets of this polyhedron. We develop some general rules about lifting facets from the uncapacitated facility location (UFL) for UHL and projecting facets from UHL to UFL. By applying these rules we get a new class of facets for UHL which dominates the inequalities in the original formulation. Thus we get a new formulation of UHL whose constraints are all facet–defining. We show its superior computational performance by benchmarking it on a well known data set.
Keywords:
integer programming, hub location, facility location, valid inequalities, facets, branch and cut
(21 S., 2000)

21. H. W. Hamacher, A. Schöbel

Design of Zone Tariff Systems in Public Transportation

Given a public transportation system represented by its stops and direct connections between stops, we consider two problems dealing with the prices for the customers: The fare problem in which subsets of stops are already aggregated to zones and "good" tariffs have to be found in the existing zone system. Closed form solutions for the fare problem are presented for three objective functions. In the zone problem the design of the zones is part of the problem. This problem is NP hard and we therefore propose three heuristics which prove to be very successful in the redesign of one of Germany's transportation systems.
(30 S., 2001)

22. D. Hietel, M. Junk, R. Keck, D. Teleaga:

The Finite-Volume-Particle Method for Conservation Laws

In the Finite-Volume-Particle Method (FVPM), the weak formulation of a hyperbolic conservation law is discretized by restricting it to a discrete set of test functions. In contrast to the usual Finite-Volume approach, the test functions are not taken as characteristic functions of the control volumes in a spatial grid, but are chosen from a partition of unity with smooth and overlapping partition functions (the particles), which can even move along prescribed velocity fields. The information exchange between particles is based on standard numerical flux functions. Geometrical information, similar to the surface area of the cell faces in the Finite-Volume Method and the corresponding normal directions are given as integral quantities of the partition functions.
After a brief derivation of the Finite-Volume-Particle Method, this work focuses on the role of the geometric coefficients in the scheme.
(16 S., 2001)

23. T. Bender, H. Hennes, J. Kalcsics, M. T. Melo, S. Nickel

Location Software and Interface with GIS and Supply Chain Management

The objective of this paper is to bridge the gap between location theory and practice. To meet this objective focus is given to the development of software capable of addressing the different needs of a wide group of users. There is a very active community on location theory encompassing many research fields such as operations research, computer science, mathematics, engineering, geography, economics and marketing. As a result, people working on facility location problems have a very diverse background and also different needs regarding the software to solve these problems. For those interested in non-commercial applications (e. g. students and researchers), the library of location algorithms (LoLA can be of considerable assistance. LoLA contains a collection of efficient algorithms for solving planar, network and discrete facility location problems. In this paper, a detailed description of the functionality of LoLA is presented. In the fields of geography and marketing, for instance, solving facility location problems requires using large amounts of demographic data. Hence, members of these groups (e. g. urban planners and sales managers) often work with geographical information too s. To address the specific needs of these users, LoLA was inked to a geographical information system (GIS) and the details of the combined functionality are described in the paper. Finally, there is a wide group of practitioners who need to solve large problems and require special purpose software with a good data interface. Many of such users can be found, for example, in the area of supply chain management (SCM). Logistics activities involved in strategic SCM include, among others, facility location planning. In this paper, the development of a commercial location software tool is also described. The too is embedded in the Advanced Planner and Optimizer SCM software developed by SAP AG, Walldorf, Germany. The paper ends with some conclusions and an outlook to future activities.
Keywords:
facility location, software development, geographical information systems, supply chain management.
(48 S., 2001)

24. H. W. Hamacher, S. A. Tjandra

Mathematical Modelling of Evacuation Problems: A State of Art

This paper details models and algorithms which can be applied to evacuation problems. While it concentrates on building evacuation many of the results are applicable also to regional evacuation. All models consider the time as main parameter, where the travel time between components of the building is part of the input and the overall evacuation time is the output. The paper distinguishes between macroscopic and microscopic evacuation models both of which are able to capture the evacuees' movement over time.
Macroscopic models are mainly used to produce good lower bounds for the evacuation time and do not consider any individual behavior during the emergency situation. These bounds can be used to analyze existing buildings or help in the design phase of planning a building. Macroscopic approaches which are based on dynamic network flow models (minimum cost dynamic flow, maximum dynamic flow, universal maximum flow, quickest path and quickest flow) are described. A special feature of the presented approach is the fact, that travel times of evacuees are not restricted to be constant, but may be density dependent. Using multicriteria optimization priority regions and blockage due to fire or smoke may be considered. It is shown how the modelling can be done using time parameter either as discrete or continuous parameter.
Microscopic models are able to model the individual evacuee's characteristics and the interaction among evacuees which influence their movement. Due to the corresponding huge amount of data one uses simulation approaches. Some probabilistic laws for individual evacuee's movement are presented. Moreover ideas to model the evacuee's movement using cellular automata (CA) and resulting software are presented.
In this paper we will focus on macroscopic models and only summarize some of the results of the microscopic approach. While most of the results are applicable to general evacuation situations, we concentrate on building evacuation.
(44 S., 2001)

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